

# Influence of spin ordering on superconducting correlations in the spin-one-half Falicov-Kimball model with Hund and Hubbard coupling

Pavol Farkašovský

Institute of Experimental Physics, Slovak Academy of Sciences  
Watsonova 47, 043 53 Košice, Slovakia

## Abstract

The generalized spin-one-half Falicov-Kimball model with Hund and Hubbard coupling is used to examine effects of spin ordering on superconducting correlations in the strongly correlated electron and spin systems. It is found that the ferromagnetic spin clusters (lines, bands, domains) suppress the superconducting correlations in the d-wave channel, while the antiferromagnetic ones have the fully opposite effect. The enhancement of the superconducting correlations due to the antiferromagnetic spin ordering is by factor 3 in the axial striped phase and even by the factor 8 in the phase segregated phase.

PACS nrs.: 71.27.+a, 71.28.+d, 74.20.-z

# 1 Introduction

The problem of formation of the charge and spin stripe order and its relation to superconductivity belongs surely to one of the most exciting ideas of contemporary solid state physics. The reason is clearly due to the observation of such an ordering in doped nickelate [1], cuprate [2] and cobaltate [3] materials, some of which constitute materials that exhibit high-temperature superconductivity. Unfortunately, despite an enormous research activity in the past the relation between the charge/spin ordering and the superconductivity is still controversial (an excellent review of relevant works dealing with this subject can be found in [4]). A considerable progress in this field has been achieved recently by Maier et al. [5] and Mondaini et al. [6]. Both groups studied the two-dimensional Hubbard model, in which stripes are introduced externally by applying a spatially varying local potential  $V_i$ , and they found a significant enhancement of the d-wave pairing correlations. However, it should be noted that the potential  $V_i$  is phenomenological and as such has no direct microscopic origin that corresponds to a degree of freedom in the actual materials. Contrary to this approach, we have presented very recently [7] an alternative model of coexistence of the charge/spin stripe order and superconductivity in the strongly correlated systems. Our approach is based on a generalized spin-one-half Falicov-Kimball model that besides the spin-independent  $U_{fd}$  as well as spin-dependent  $J_z$  Coulomb interaction between the localized  $f$  and itinerant  $d$  electrons takes into account the Hubbard interaction between  $d$  ( $f$ ) electrons of opposite spins. It is found that in the presence of all above mentioned interactions the model stabilizes three basic types of charge/spin ordering, and namely, the axial striped phases, the regular  $n$ -molecular phases and the phase separated states. It is shown that the  $d$ -wave pairing correlations are enhanced within the axial striped and phase separated states, but not in the regular phases. Moreover, it was found that the antiferromagnetic spin arrangement within

the chains further enhances the  $d$ -wave pairing correlations, while the ferromagnetic one has a fully opposite effect. This fact indicates that the type of spin ordering plays an important role in the mechanism of stabilization of superconductivity in strongly correlated systems and thus we have decided, within the current paper, to examine this phenomenon in more detail.

## 2 Model

The Hamiltonian of the model considered in this paper has the form

$$\begin{aligned}
H = & -t \sum_{\langle i,j \rangle \sigma} d_{i\sigma}^+ d_{j\sigma} + U_{fd} \sum_{i\sigma\sigma'} f_{i\sigma}^+ f_{i\sigma} d_{i\sigma'}^+ d_{i\sigma'} + J_z \sum_{i\sigma} (f_{i-\sigma}^+ f_{i-\sigma} - f_{i\sigma}^+ f_{i\sigma}) d_{i\sigma}^+ d_{i\sigma} \\
& + U_{dd} \sum_i d_{i\uparrow}^+ d_{i\uparrow} d_{i\downarrow}^+ d_{i\downarrow}, \tag{1}
\end{aligned}$$

where  $f_{i\sigma}^+, f_{i\sigma}$  are the creation and annihilation operators for an electron of spin  $\sigma = \uparrow, \downarrow$  in the localized state at lattice site  $i$  and  $d_{i\sigma}^+, d_{i\sigma}$  are the creation and annihilation operators of the itinerant electrons in the  $d$ -band Wannier state at site  $i$ .

The first term of (1) is the kinetic energy corresponding to quantum-mechanical hopping of the itinerant  $d$  electrons between sites  $i$  and  $j$ . These intersite hopping transitions are described by the matrix elements  $t_{ij}$ , which are  $-t$  if  $i$  and  $j$  are the nearest neighbours and zero otherwise. The second term represents the on-site Coulomb interaction between the  $d$ -band electrons with density  $n_d = N_d/L = \frac{1}{L} \sum_{i\sigma} d_{i\sigma}^+ d_{i\sigma}$  and the localized  $f$  electrons with density  $n_f = N_f/L = \frac{1}{L} \sum_{i\sigma} f_{i\sigma}^+ f_{i\sigma}$ , where  $L$  is the number of lattice sites. The third term is the above mentioned anisotropic, spin-dependent local interaction of the Ising type between the localized and itinerant electrons that reflects the Hund's rule force. And finally, the last term is the ordinary Hubbard interaction term for the itinerant electrons from the  $d$  band. Moreover, it is assumed that the on-site Coulomb interaction between  $f$  electrons is infinite and so the double occupancy of  $f$  orbitals is forbidden.

This model has several different physical interpretations that depend on its application. As was already mentioned above, it can be considered as the spin-one-half Falicov-Kimball model extended by the Hund and Hubbard interaction term. On the other hand, it can be also considered as the Hubbard model in the external potential generated by the spin-independent Falicov-Kimball term and the anisotropic spin-dependent Hund term. Very popular interpretation of the model Hamiltonian (1) is its ( $U_{dd} = 0$ ) version that has been introduced by Lemanski [8] who considered it as the minimal model of charge and magnetic ordering in coupled electron and spin systems. Its attraction consists in this that without the Hubbard interaction term ( $U_{dd} = 0$ ) the Hamiltonian (1) can be reduced to the single particle Hamiltonian

$$H = \sum_{ij\sigma} h_{ij}^{(\nu)} d_{i\sigma}^+ d_{j\sigma}, \quad (2)$$

where  $h_{ij}^{(\nu)} = t_{ij} + (U_{fd}w_i + J_z\nu s_i)\delta_{ij}$ ,  $w_i = w_{i\uparrow} + w_{i\downarrow} = 0, 1$ ,  $s_i = w_{i\uparrow} - w_{i\downarrow} = -1, 1$  and  $\nu = \pm 1$ . Thus for a given  $f$ -electron  $w = \{w_1, w_2, \dots, w_L\}$  and spin configuration  $s = \{s_1, s_2, \dots, s_L\}$  the investigation of the model (2) is reduced to the investigation of the spectrum of  $h^{(\nu)}$  for different  $f$  electron/spin distributions. This can be performed exactly, over the full set of  $f$ -electron/spin distributions or approximatively. Numerical solutions obtained within so called restricted set phase diagram method [8,9] as well as our well controlled gradient method [10,11] showed that this model is able to describe various types of charge and spin orderings observed experimentally in strongly correlated systems, including the diagonal and axial charge stripes with the antiferromagnetic or ferromagnetic arrangement of spins within the lines. Moreover, using the exact diagonalization calculations [11] on small clusters ( $L = 16$ ) and the Projector Quantum-Monte-Carlo Method [7] on larger clusters ( $L \leq 64$ ), we have found that in the strong coupling  $U_{fd}$  limit ( $U_{fd} \geq 4$ ) the ground states of the model (1) found for  $U_{dd} = 0$  persist as ground states also for nonzero  $U_{dd}$ , up to relatively large values ( $U_{dd}^c \sim 3$ ). This fact allows us to avoid the exhaustive numerical

calculations on the full model Hamiltonian (1) and represent its ground states directly by a set of ground states of numerically much simpler single particle Hamiltonian (2), at least in the strong coupling  $U_{fd}$  limit and  $U_{dd} < U_{dd}^c$ . For these ground states we then calculate the superconducting correlation functions of the full model Hamiltonian with  $U_{dd} > 0$  by the Projector Quantum-Monte-Carlo Method [12].

In particular we calculate the superconducting correlation function with  $d_{x^2-y^2}$  wave symmetry defined as [13]

$$C_d(r) = \frac{1}{L} \sum_{i, \delta, \delta'} g_\delta g_{\delta'} \langle d_{i\uparrow}^+ d_{i+\delta\downarrow}^+ d_{i+\delta'+r\downarrow} d_{i+r\uparrow} \rangle, \quad (3)$$

where the factors  $g_\delta, g_{\delta'}$  are 1 in x-direction and -1 in y-direction and the sums with respect to  $\delta, \delta'$  are independent sums over the nearest neighbors of site  $i$ .

However, on small clusters the above defined correlation function is not a good measure for superconducting correlations, since contains also contributions from the one particle correlation functions

$$C_0^\sigma(r) = \frac{1}{L} \sum_i \langle d_{i\sigma}^+ d_{i+r\sigma} \rangle, \quad (4)$$

that yield nonzero contributions to  $C_d(r)$  even in the noninteracting case.

For this reason we use as the true measure for superconductivity the vertex correlation function

$$C_d^v(r) = C_d(r) - \sum_{\delta, \delta'} g_\delta g_{\delta'} C_0^\uparrow(r) C_0^\downarrow(r + \delta - \delta'), \quad (5)$$

and its average

$$C_d^v = \frac{1}{L} \sum_i C_d^v(i). \quad (6)$$

### 3 Results and discussion

As mentioned above, the main goal of the present paper is to investigate the influence of the spin ordering on the superconducting correlations in the ground state of the model Hamiltonian (1). To fulfill this goal we have performed exhaustive numerical studies of the model for two selected values of  $f$ -electron fillings  $N_f$  ( $N_f = L/2$  and  $N_f = L$ ) and the complete set of even  $d$ -electron fillings  $N_d$  on the cluster of  $L = 8 \times 8$  sites. The reasons for such a selection of  $N_f$  values are following. The previous numerical results [11] obtained for the case  $N_f = L/2$  showed that the ground states of the model (2) in this case are mainly the segregated or axial striped charge phases. However, according to our very recent results [7] these configuration types enhance the  $d$ -wave pairing correlations in the  $d_{x^2-y^2}$  channel of the full model Hamiltonian (1) and thus they are ideal candidates for the examination of effects of spin ordering on this charge induced superconducting state. In addition, it was found [11] that for both charge phases, the segregated one as well as the axial striped one, there are many different spin arrangements that minimize the ground state energy of the model at different  $d$ -electron fillings  $N_d$ . Thus it is possible to study simultaneously (by changing only one parameter  $N_d$ ) the influence of the spin ordering and the  $d$ -electron doping on superconducting correlations. On the other hand the case of  $N_f = L$  is of special importance for this reason that in this limit our model reduces on a simple spin-fermion model with an additional  $U_{dd}$  interaction.

Let us first discuss results obtained for  $N_f = L/2$ . In Fig. 1 and Fig. 2 we present typical examples of ground states, that minimize the ground state energy of the model Hamiltonian (2) for  $U_{fd} = 4$ ,  $J_z = 0.5$  and  $U_{dd} = 0$ . One can see that for both the axial striped as well as phase segregated phase there are several different spin arrangements that allow us to test the impact of spin ordering on the superconducting correlations. Before this let us discuss in more detail these configurations types. In all

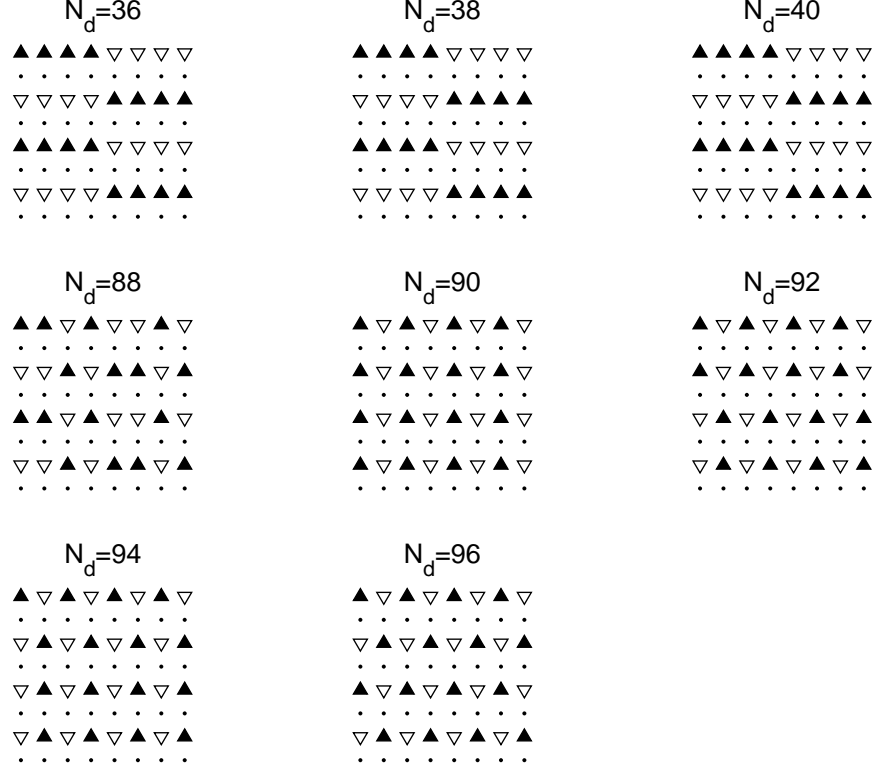


Figure 1: The axial striped ground states of the model (1) obtained for  $U_{fd} = 4, J_z = 0.5, U_{dd} = 0$  and  $N_f = L/2$  on the  $L = 8 \times 8$  site cluster. Here the spin up (down) of the  $f$  electron is represented by a filled regular triangle (open inverted triangle).

examined cases the ground states of the model are non-polarized ( $S_z = 0$ ) for both the axial striped and segregated phase. For the axial striped phase the one dimensional chains are formed by (i) the four-spin ferromagnetic clusters of opposite orientation, (ii) the mixture of two-spin ferromagnetic clusters and  $\uparrow\downarrow$  or  $\downarrow\uparrow$  pattern and (iii) the classical Neel state pattern  $\uparrow\downarrow \dots \uparrow\downarrow$ . A similar situation we can observe also in the phase segregated phase. Here we can find (i) the antiparallel ferromagnetic chains (bands), (ii) the antiparallel small or large ferromagnetic domains and (iii) some intermediate phases.

The average vertex correlation functions  $C_d^v$  corresponding to these ground states

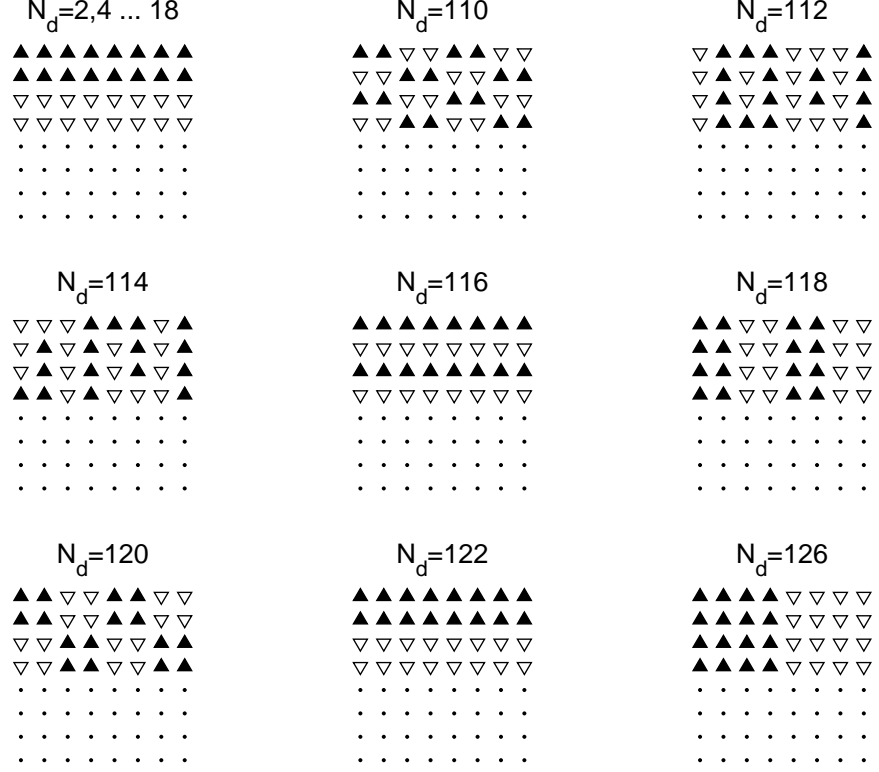


Figure 2: The phase segregated ground states of the model (1) obtained for  $U_{fd} = 4$ ,  $J_z = 0.5$ ,  $U_{dd} = 0$  and  $N_f = L/2$  on the  $L = 8 \times 8$  site cluster.

are displayed in Fig. 3 (for the axial striped phase) and Fig. 4 (for the segregated phase). One can see that in the case of axial striped phases the superconducting correlations are enhanced the most significantly for the chessboard distribution of spins. All deviation from this state in the meaning of forming the ferromagnetic clusters or an improper extension of the chessboard structure in the y-direction suppress the superconducting correlations in the  $d$ -wave channel. Moreover, there is observed an obvious relation between the size of ferromagnetic clusters (domains) and the superconducting correlations, the largest ferromagnetic clusters, the smallest vertex correlations. However, the vertex correlations in Fig. 3 are displayed for different  $d$ -electron fillings and



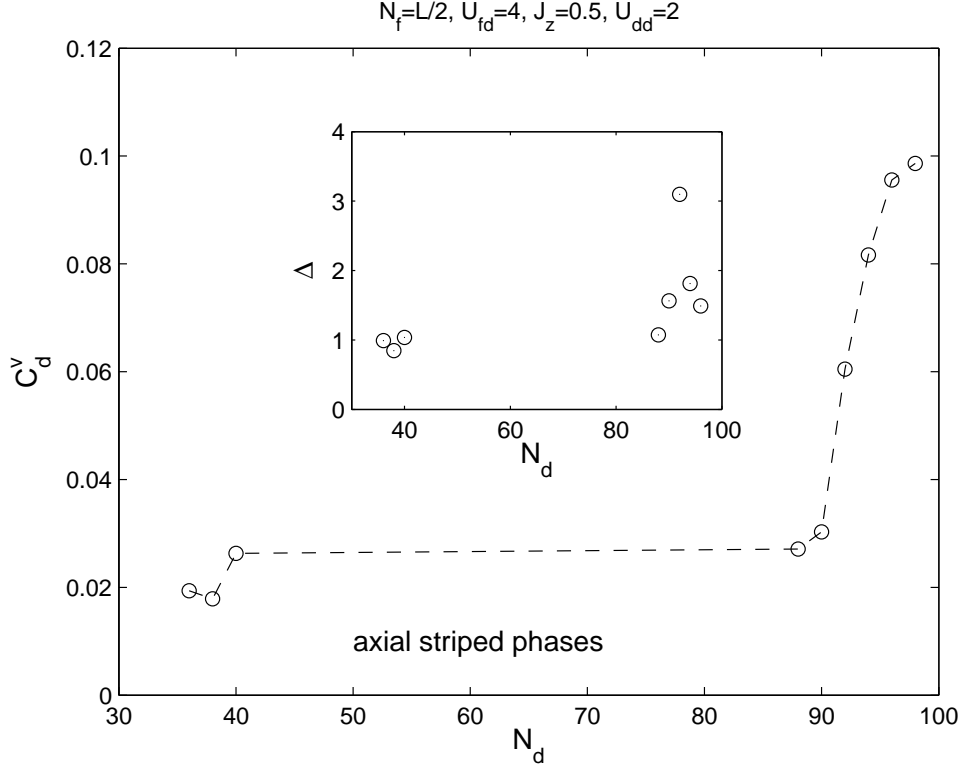


Figure 3: Average vertex correlation function  $C_d^v$  with  $d_{x^2-y^2}$ -symmetry calculated for corresponding ground states from Fig. 1. The inset shows the enhancement  $\Delta$  corresponding to the ratio of the average vertex correlation functions with and without the Ising coupling  $J_z$ ,  $\Delta = C_d^v(J_z = 0.5)/C_d^v(J_z = 0)$ .

thus it is questionable if the enhancement/suppression of vertex correlations is a net effect of different spin orderings, or it is, at least partially, produced by the  $d$ -electron doping. To separate contributions to  $C_d^v$  from  $N_d$  and  $J_z$  we have plotted in the inset to Fig. 3 the ratio of the average vertex correlation functions with and without the Ising coupling  $J_z$ ,  $\Delta = C_d^v(J_z = 0.5)/C_d^v(J_z = 0)$ . These results show that for  $N_d = 36, 38, 40$ , where the ground states are identical, the ratio  $\Delta$  depends only very weakly on  $N_d$  what documents that the effects of electron doping on superconducting correlations are not very important. On the other hand the results from the opposite limit  $N_d > L/2$  show the strong enhancement of  $\Delta$  in the region where the ground states are different non-polarized spin orderings without or with small ferromagnetic

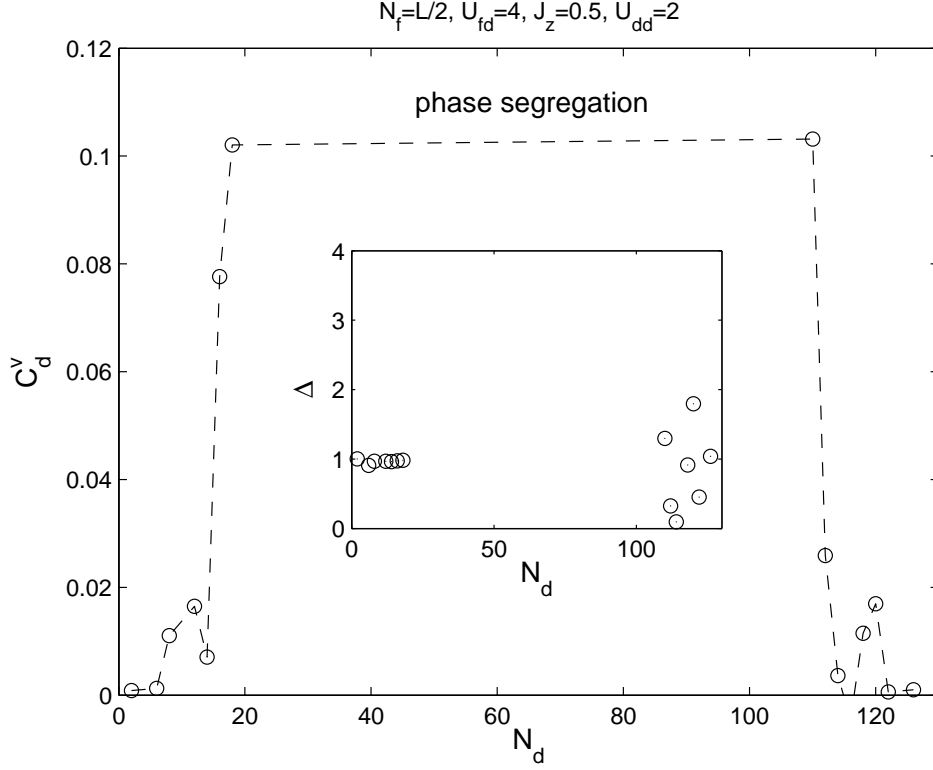


Figure 4: Average vertex correlation function  $C_d^v$  and the enhancement  $\Delta$  calculated for corresponding ground states from Fig. 2.

clusters of length two, what clearly demonstrates the impact of such a spin ordering on the superconducting correlations.

A slightly different behaviour of the model is observed in the segregated phase (see Fig. 4). Here the superconducting correlations are strongly enhanced going with  $N_d$  from 2 to 18. Since the spin ordering in all these cases is identical, the enhancement of superconducting correlations in this region is obviously a net effect of electron doping. In the opposite limit  $N_d > L/2$  the superconducting correlations are enhanced for the smallest ferromagnetic clusters and they are strongly suppressed with the increasing size of ferromagnetic clusters (domains). In this region the increase (decrease) in  $C_d^v$  does not fully coincide with increase (decrease) in  $\Delta$  what indicates that the enhancement of the superconducting correlations for  $N_d > L/2$  is the combined effect

of spin ordering and the  $d$ -electron doping.

Let us now turn our attention to the case  $N_f = L$ . The ground states of the single particle Hamiltonian (2), that are used as the approximative ground states of the full model Hamiltonian (1) are displayed in Fig. 5. Obviously there are some general

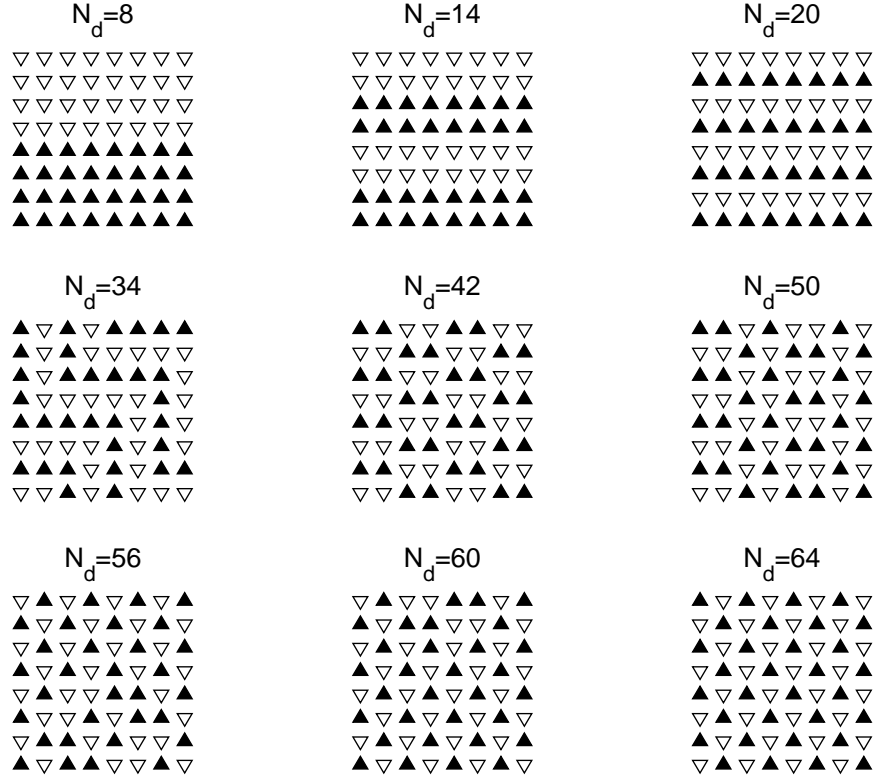


Figure 5: Ground states of the model (1) obtained for  $U_{fd} = 4, J_z = 0.5, U_{dd} = 0$  and  $N_f = L$  on the  $L = 8 \times 8$  site cluster.

trends in the spin ordering going with  $N_d$  from 0 to  $L$ . For  $N_d$  small (e.g.,  $N_d = 8$ ) the ground state is formed by two large antiparallel ferromagnetic domains, that transforms with increasing  $d$ -electron filling  $N_d$  on antiparallel ferromagnetic bands (e.g.,  $N_d = 14$ ) and finally on antiparallel ferromagnetic chains (e.g.,  $N_d = 20$ ). Then follows the region of perturbed antiparallel ferromagnetic chains (e.g.,  $N_d = 34$ ) and

the region of regularly distributed pairs of up and down spins (e.g.,  $N_d = 42$ ). The next phases can be considered as a mixture of this regular phase and the chessboard phase (e.g.,  $N_d = 50$ ). Then follows the region of incompletely developed chessboard phase (e.g.,  $N_d = 56$ ), which ends with the prefect developed chessboard structure at  $N_d = L/2$ .

The average vertex correlation functions  $C_d^v$  corresponding to these ground states are displayed in Fig. 6. It is seen that the superconducting correlations are negligible

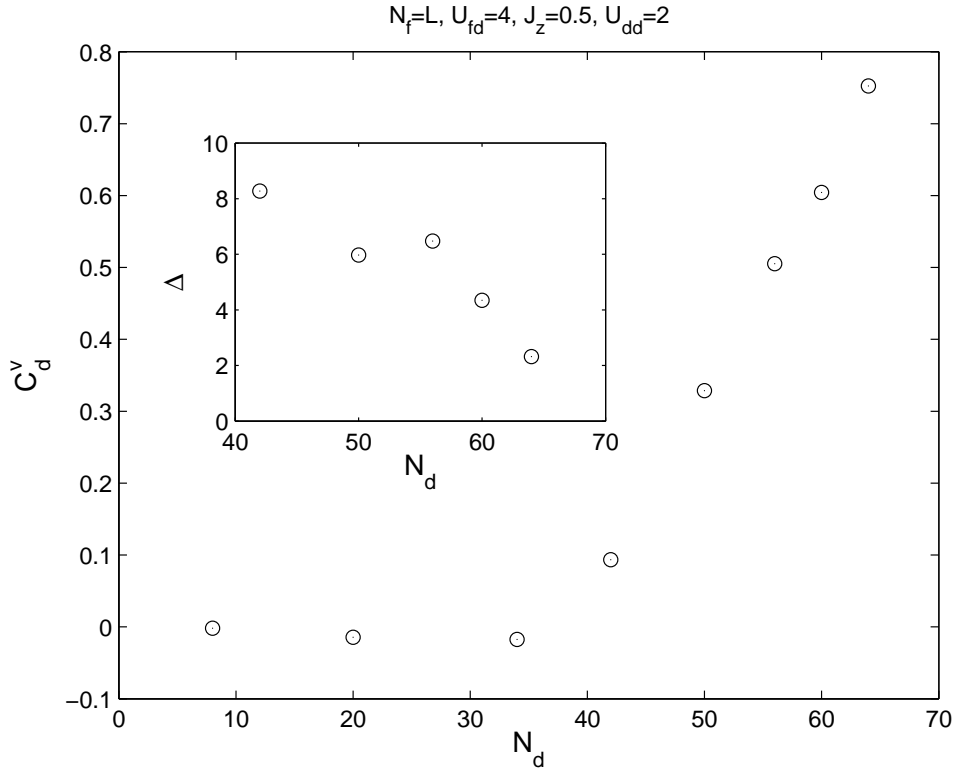


Figure 6: Average vertex correlation function  $C_d^v$  and the enhancement  $\Delta$  calculated for corresponding ground states from Fig. 5.

in phases that are composed of large antiparallel ferromagnetic domains, bands and chains what is fully consistent with our above discussed results and conclusions. The superconducting correlations start to increase from the region of stability of regular phases, what is also in accordance with our above mentioned conclusions, since these

phases are formed by small antiparallel ferromagnetic clusters of length two. In the region of formation of the chessboard structure, the vertex correlation function is dramatically enhanced and reaches its maximum for the perfect ordered chessboard phase (for  $N_d > L/2$  the vertex correlation function  $C_d^v$  exhibits the mirror symmetry). The same behaviour exhibits also the ratio  $\Delta$  that is enhanced by factor 6-8 in comparison to the  $J_z = 0$  case, what clearly documents the strong effects of spin ordering on superconducting correlations in coupled electron and spin systems.

In summary, we have used the generalized spin-one-half Falicov-Kimball model with Hund and Hubbard coupling to study effects of spin ordering on superconducting correlations in the axial striped and phase segregated state. It was found that the ferromagnetic spin clusters (lines, bands, domains) suppress the superconducting correlations in the d-wave channel, while the antiferromagnetic ones have the fully opposite effect. The enhancement of the superconducting correlations due to the antiferromagnetic spin ordering is by factor 3 in the axial striped phase and even by the factor 8 in the phase segregated phase.

This work was supported by Slovak Research and Development Agency (APVV) under Grant APVV-0097-12 and ERDF EU Grants under the contract No. ITMS 26220120005 and ITMS26210120002.

## References

- [1] C. H. Chen, S.-W. Cheong and A. S. Cooper, Phys. Rev. Lett. **71**, 2461 (1993); J. M. Tranquada, D. J. Buttrey, V. Sachan and J. E. Lorenzo, Phys. Rev. Lett. **73**, 1003 (1994); Phys. Rev. B **52**, 3581 (1995); V. Sachan *et al.*, *ibid.* **51**, 12742 (1995).
- [2] J. M. Tranquada, B. J. Sternlieb, J. D. Axe, Y. Nakamura and S. Uchida, Nature (London) **375**, 561 (1995); Phys. Rev. B **54**, 7489 (1996); Phys. Rev. Lett. **78**, 338 (1997); H. A. Mook, P. Dai and F. Dogan, Phys. Rev. Lett. **88**, 097004 (2002);
- [3] K. Takada, H. Sakurai, E. Takayama-Muromachi, F. Izumi, R. Dilanian, and T. Sasaki, Nature (London) **422**, 53 (2003)
- [4] A.M. Oles, Acta Physica Polonica B **121**, 752 (2012).
- [5] T.A. Maier, G. Alvarez, M. Summers and T.C. Schulthess, Phys. Rev. Lett. **104**, 247001 (2010).
- [6] R. Mondaini, T. Ying, T. Paiva and R.T. Scalettar, Phys. Rev. B **86**, 184506 (2012).
- [7] P. Farkašovský, EPL **115**, 37006 (2016).
- [8] R. Lemanski, Phys. Rev. B **71**, 035107 (2005).
- [9] R. Lemanski and J. Wrzodak, Phys. Rev. B **78**, 085118 (2008).
- [10] P. Farkašovský and H. Čenčariková, Eur. Phys. J. B **47**, 517 (2005).
- [11] H. Čenčariková and P. Farkašovský, phys. stat. sol. (b) **245**, 2593 (2008).
- [12] M. Imada and Y. Hatsugai, J. Phys. Soc. Jpn. **58**, 3752 (1989).

- [13] M. Fettes, I. Morgenstern and T. Husslein, Computer Physics Communications **106**, 1 (1997).